

2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester
13533-05-6 | DTXSID5050397

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.27e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 3.63e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Decanal</div> <div>Measured: 2.19e-02</div> <div>Predicted: 1.51e-01</div>	<div>Image not found</div> <div>1-Octanethiol</div> <div>Measured: 1.26e-01</div> <div>Predicted: 3.49e-01</div>	<div>Image not found</div> <div>Tetraethylenepentamine</div> <div>Measured: 1.18e-03</div> <div>Predicted: 1.09e-06</div>
<div>Image not found</div> <div>Heptanal</div> <div>Measured: 2.50e-01</div> <div>Predicted: 2.33</div>	<div>Image not found</div> <div>Quinuclidine</div> <div>Measured: 107</div> <div>Predicted: 2.06</div>	